Massively Parallel Molecular–Continuum Simulations with the Macro-Micro-Coupling Tool

HYBRID 2013

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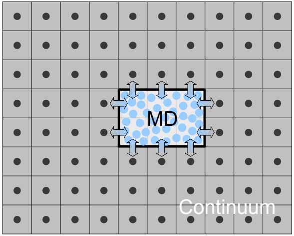
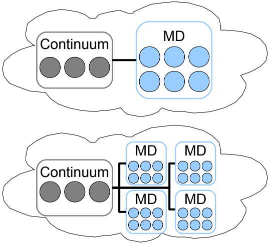
07.03.2013

Contents

Challenges: Physics & Distributed Computing



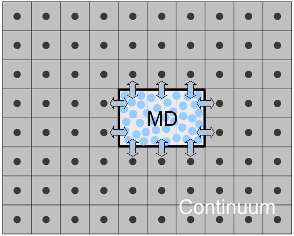


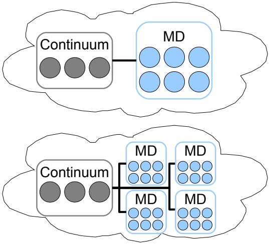
- Correct physical description at molecular–continuum interface
- Simple & fast testing of new coupling schemes

- Statistical noise on MD data[1] $\rightarrow$ sampling
- Flexibility
- (Massively) Parallel implementation

[1] N.G. Hadjiconstantinou, A.L. Garcia, M.Z. Bazant and G. He, Statistical error in particle simulations of hydrodynamic phenomena. J. Comput. Phys. 187, pp. 274–297, 2003.

Challenges: Physics & Distributed Computing





- Correct physical description at molecular–continuum interface
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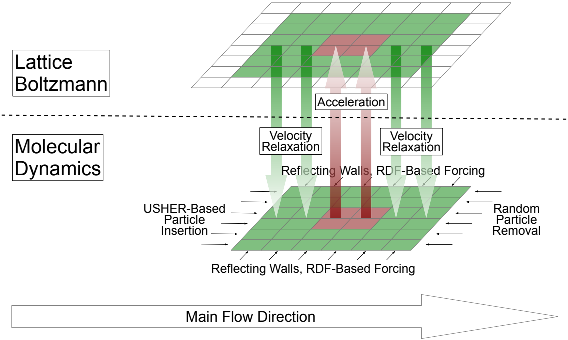
Goal: Provide a Tool for Flexible Parallel Mesh–Particle Multiscale Coupling

[1] N.G. Hadjiconstantinou, A.L. Garcia, M.Z. Bazant and G. He, Statistical error in particle simulations of hydrodynamic phenomena. J. Comput. Phys. 187, pp. 274–297, 2003.

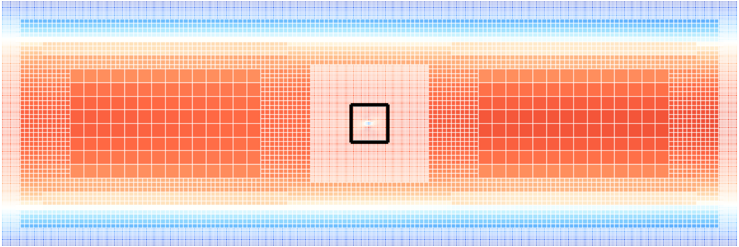
From Prototype To Coupling Software (1)



- State-based coupling, following the coupling approach of Dupuis et al.[1]
- Channel flows

[1] A. Dupuis, E.M. Kotsalis and P. Koumoutsakos, Coupling lattice Boltzmann and molecular dynamics models for dense fluids. Phys. Rev. E 75 (046704), 2007.

From Prototype To Coupling Software (2)



- Coupling of Mardyn[1] and Peano's Lattice Boltzmann component[2]
  - MD: 3D, LB: 2D
  - MD: Velocity relaxation in overlap regions
  - MD: RDF-based boundary forces vs. periodic boundaries
  - LB: Forcing terms for momentum exchange

[1] M. Buchholz, Framework zur Parallelisierung von Molekulardynamiksimulationen in verfahrenstechnischen Anwendungen. PhD thesis. Institut für Informatik, Technische Universität München. Verlag Dr. Hut, München, 2010.

[2] P. Neumann and T. Neckel, A dynamic mesh refinement technique for Lattice Boltzmann simulations on octree-like grids. Comput. Mech., 51(2):237–253, 2013.

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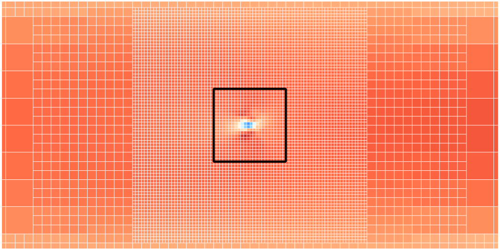

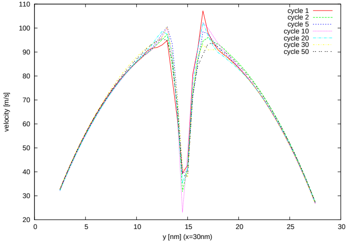

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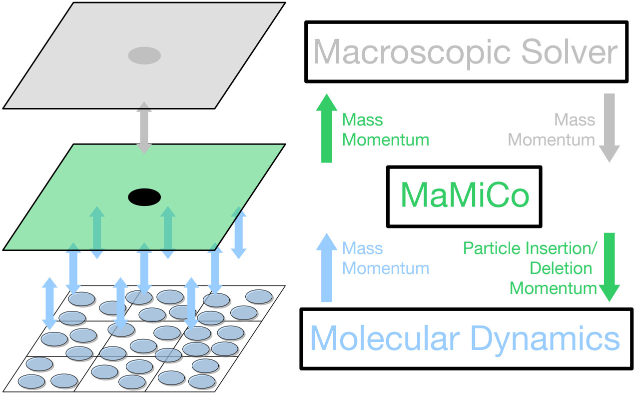
The Macro–Micro Coupling Tool (MaMiCo)[1]



1 P. Neumann and N. Tchipev, A Coupling Tool for Parallel Molecular Dynamics–Continuum Simulations. Proceedings of the 11th International Symposium on Distributed and Parallel Computing, München, 2012.

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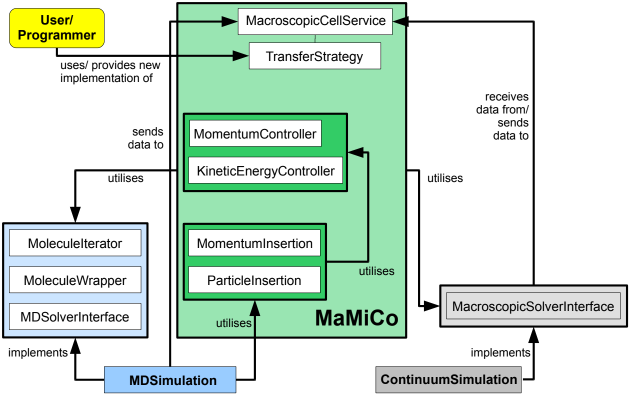

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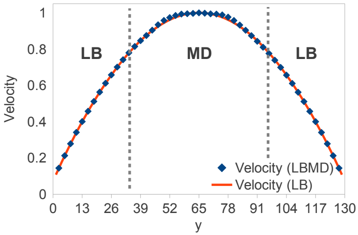
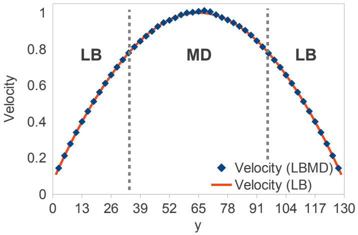
Validation



D-linear interpolation



Second-order interpolation

- Fully three-dimensional state-based coupling
- Channel flow
- LB:
  - $54 \times 54 \times 54$ cells
  - $dx = 2.5$
- MD:
  - S.-c. LJ: $\epsilon = 1.0$, $\sigma = 1.0$
  - $\sim 10^5$ molecules in a cube, placed in the channel center
  - periodic boundaries + buffer regions

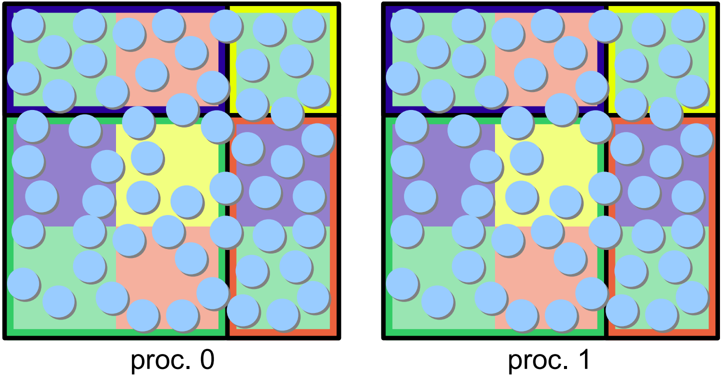
Runtimes: Mass & Momentum Insertion

Scenario	Runtime (s)	Timesteps/ Particle insertion	Timesteps/ Momentum insertion
MD($n = 0.40$) (2D)	23.5	0	0
MD($n = 0.78$) (2D)	46.6	0	0
Test A (2D)	55.9	30	0
MD($n = 0.80$) (2D)	48.0	0	0
Test B ($n = 0.80$) (2D)	54.8	0	30
MD($n = 0.40$) (3D)	92.1	0	0
MD($n = 0.78$) (3D)	166.7	0	0
Test A (3D)	268.4	15	0
MD($n = 0.80$) (3D)	167.7	0	0
Test B ($n = 0.80$) (3D)	175.2	0	15

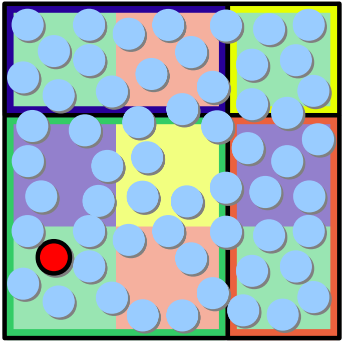
Test A: $n = 0.40 \rightarrow n = 0.78$

Test B: $v = 1.0 \rightarrow v = 2.0$

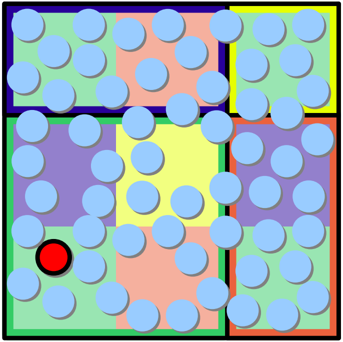
Parallel Particle Insertion



Parallel Particle Insertion

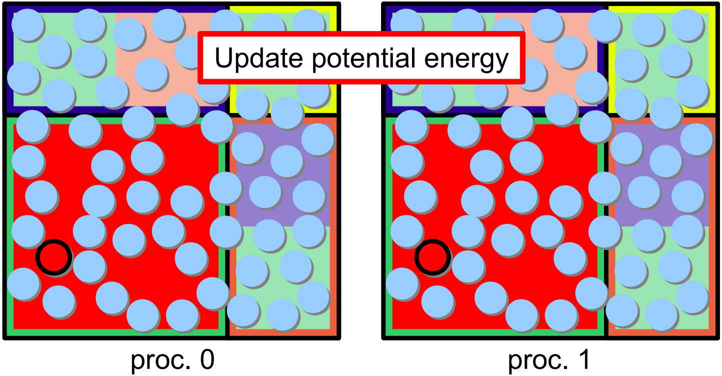


proc. 0



proc. 1

Parallel Particle Insertion



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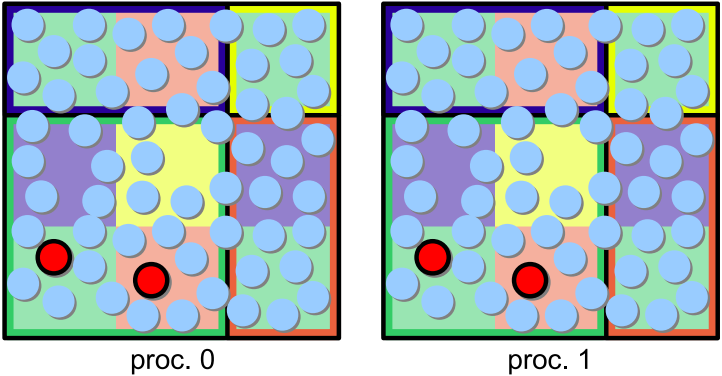

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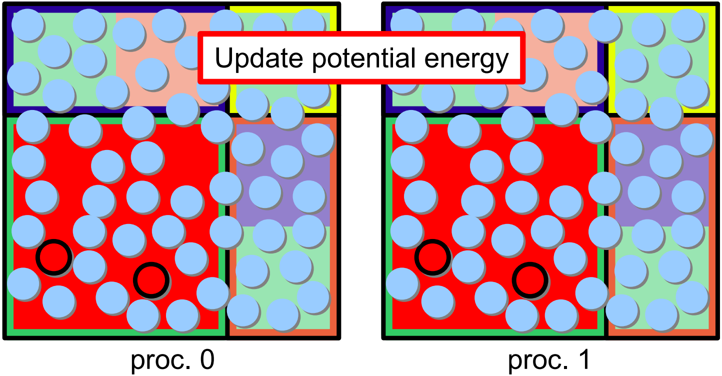

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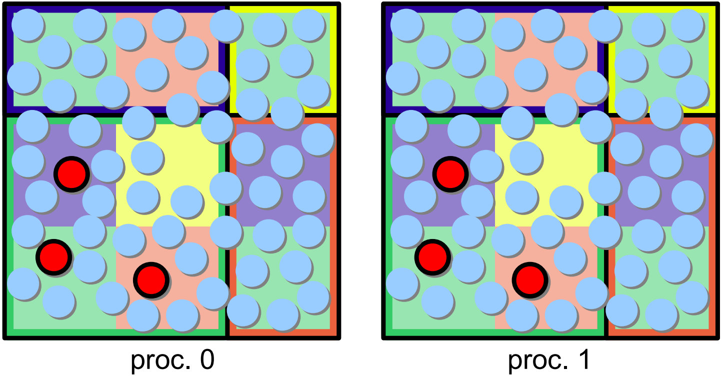

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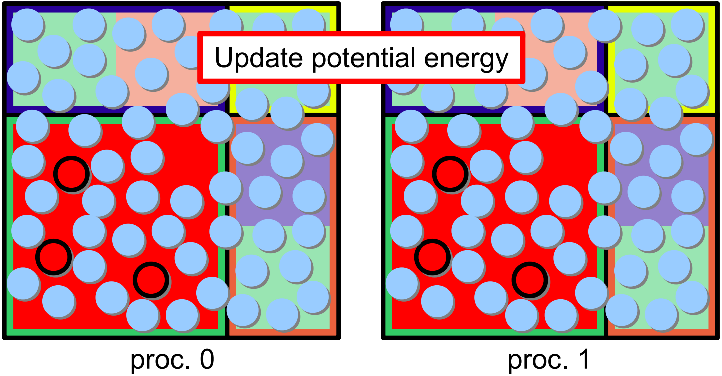

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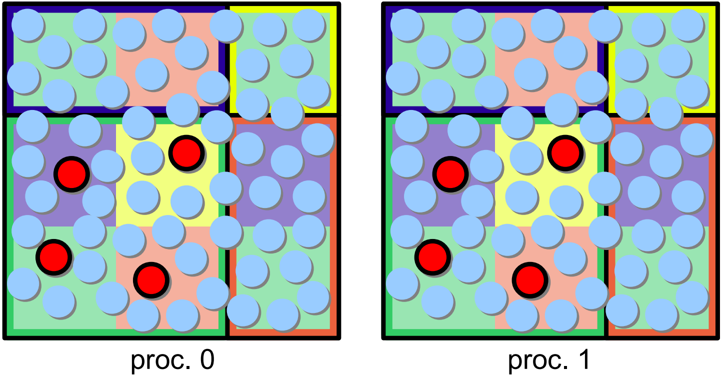

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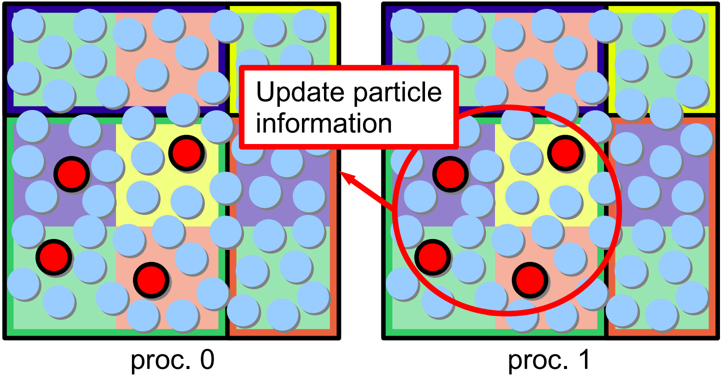

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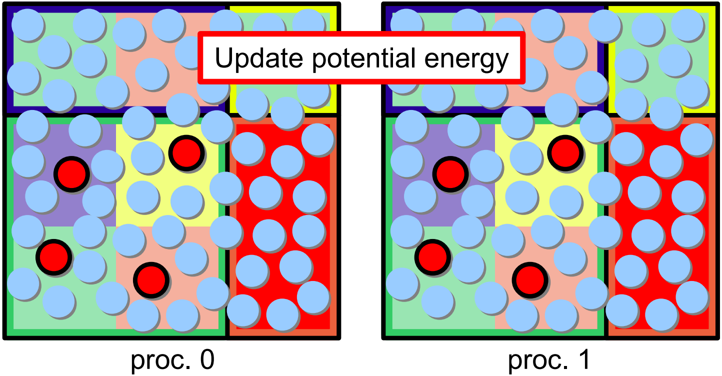
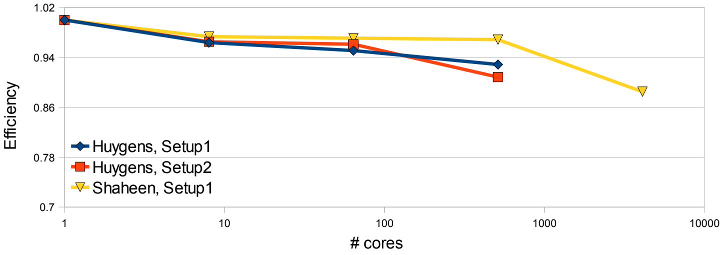
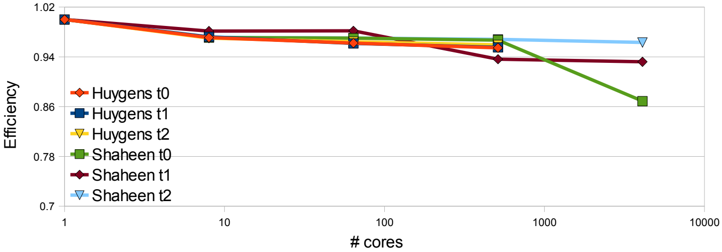
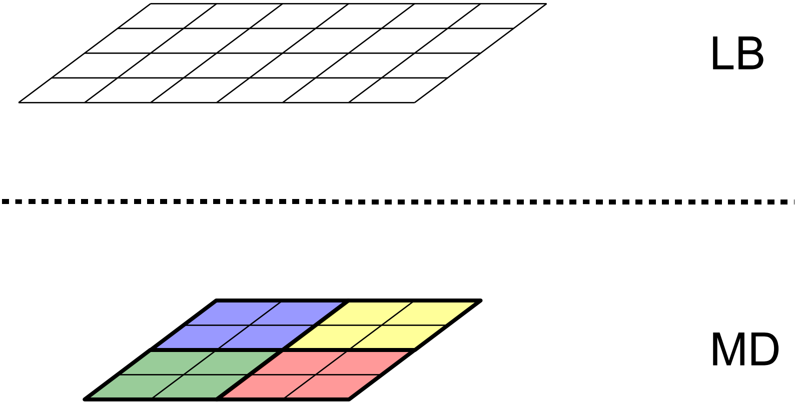


Parallel Particle Insertion: Weak Scaling (3D)





Parallelisation: Exchange MD↔LB



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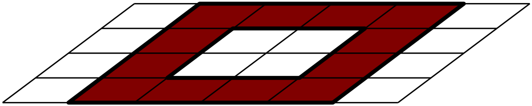
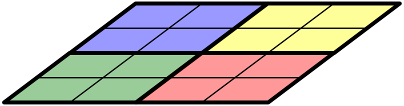


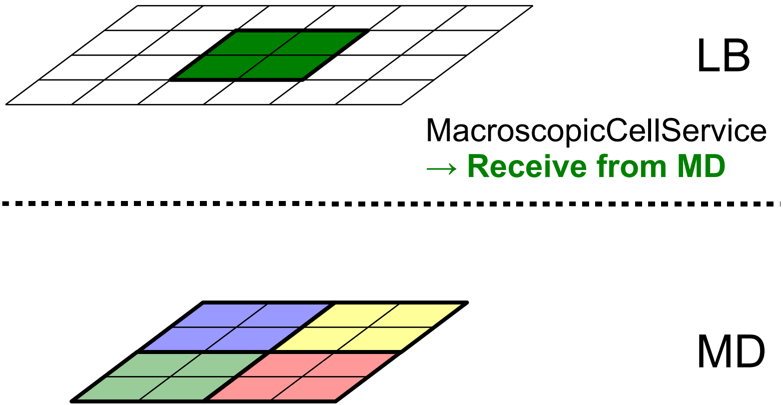
LB

MacroscopicCellService
→ **Send to MD**



MD

Parallelisation: Exchange MD↔LB



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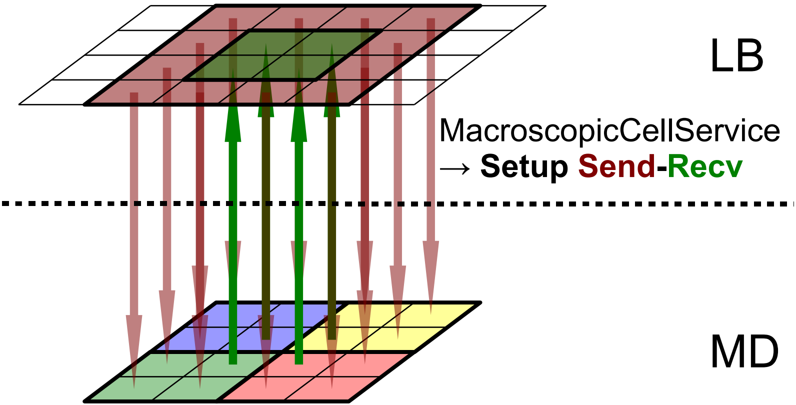
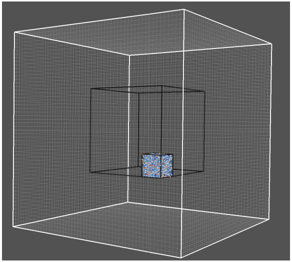
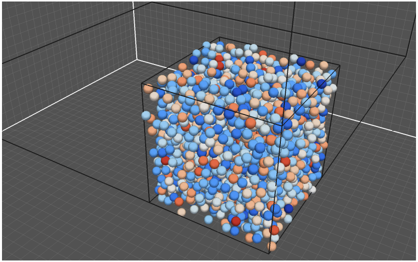


MD–LB Channel Flow: Strong Scaling





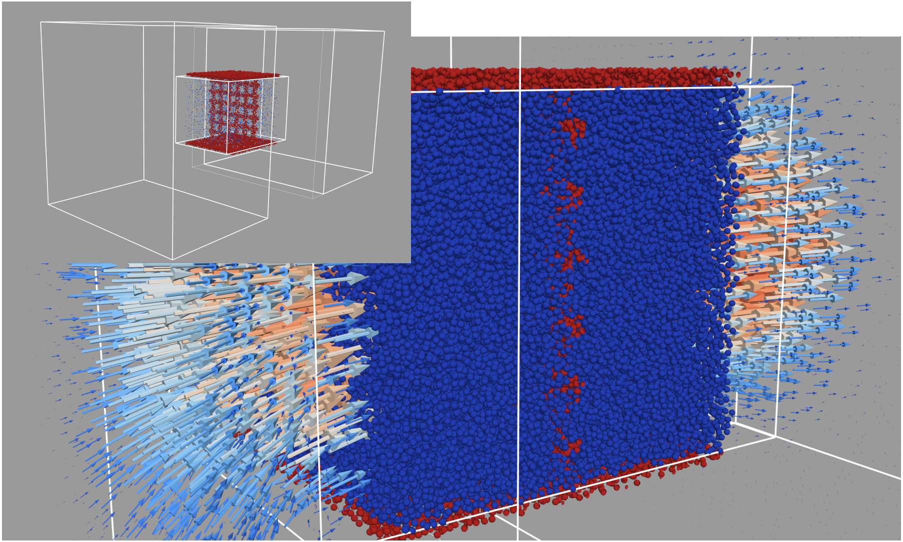
- LB: sequential, $54 \times 54 \times 54$ cells
- MD: parallel, 1 000 000 molecules $\leftrightarrow$ $24 \times 24 \times 24$ LB cells
- Retain average density in outermost macroscopic cells
  $\rightarrow$ USHER
- One coupling cycle: 1 LB step, 100 MD steps

MD–LB Channel Flow: Strong Scaling

Proc.	Shaheen		Huygens	
	MD-LB	MD	MD-LB	MD
1	1.0	1.0	1.0	1.0
8	7.2	7.3	7.3	6.9
64	46.0	49.6	45.7	45.3
512	244.0	321.0	235.5	249.7
1728	484.4	814.5	456.7	494.7

- LB: sequential, $54 \times 54 \times 54$ cells
- MD: parallel, 1 000 000 molecules $\leftrightarrow$ $24 \times 24 \times 24$ LB cells
- Retain average density in outermost macroscopic cells $\rightarrow$ USHER
- One coupling cycle: 1 LB step, 100 MD steps

Outlook: Filter Simulations



Conclusion & Outlook

Conclusion: A coupling tool

- which provides the ingredients for hybrid molecular–continuum simulations
- takes care of distributed memory parallelisation of hybrid schemes
- shows good scaling behaviour on core counts up to $O(1000)$

Outlook:

- Filter simulations
- Open boundaries
- Other MD/ CFD solvers for coupling

Thanks to:
Peter Hoffmann
Nikola Tchipev